Combinatorial nuclear level density
by a Monte Carlo method

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Abstract

We present a new combinatorial method for the calculation of the nuclear level density. It is based on a Monte Carlo technique, in order to avoid a direct counting procedure which is generally impracticable for high-A nuclei. The Monte Carlo simulation, making use of the Metropolis sampling scheme, allows a computationally fast estimate of the level density for many fermion systems in large shell model spaces. We emphasize the advantages of this Monte Carlo approach, particularly concerning the prediction of the spin and parity distributions of the excited states, and compare our results with those derived from a traditional combinatorial or a statistical method. Such a Monte Carlo technique seems very promising to determine accurate level densities in a large energy range for nuclear reaction calculations.

1 Introduction

The density of nuclear levels provides information about the structure of highly excited nuclei, and is also a basic quantity in nuclear reaction theory. For many years, measurements of nuclear level densities have been interpreted in the framework of an infinite Fermi gas model (see e.g. [1]), and most calculations have employed the well-known Bethe formula [2] since it predicts a general trend in reasonable accordance with experimental data (i.e., an approximately exponential increase of the level density with both the excitation energy and the mass number). The Bethe formula is based on the statistical model (see e.g. [3, 4]), and involves three major assumptions: (*i*) the independent particles assumption, allowing to write a nuclear partition function in a simple form using single-particle energies, (*ii*) an equidistant spacing of the single-particle states near the Fermi level, and (*iii*) the saddle-point approximation used to calculate the inverse Laplace transform of the partition function. As a result of assumptions (*i*) and (*ii*), this simple model includes neither odd-even effects nor shell effects, and it has been pointed out in ref. [5] that assumption (*iii*) is not very good in the nuclear case. Therefore, various phenomenological modifications of this simple formula have been proposed for use in practical calculations to account for these effects (see ref. [6] for a recent review). These are mostly based on the ad-hoc hypothesis that the same functional form of the energy dependence as in the equidistant-level case is valid, some free parameter(s) being introduced in order to match experimental results. In the Newton-Cameron shifted Fermi-gas model [7, 8], the odd-even effects are included by means of a pairing energy shift. The effective excitation energy is reduced by the conventional pairing energy for the odd-mass and even-even nuclei, resulting in a lower level density. The pairing energy is determined from experimental odd-even mass differences, and the level density parameter a is the only adjustable parameter. This model is able to describe experiments in a narrow energy interval around the neutron binding energy, most experimental data being extracted from the neutron resonances, but it does not allow to extrapolate the value of the level density in either the low- or the high-energy regions. This means that shell effects are not properly taken into account.

In order to solve this problem, Gilbert and Cameron [9] proposed another formula (the composed four-parameter formula) which combines the shifted Fermi gas formula at high excitation energies with a constant temperature formula (see e.g. [10]) for lower energies. By fitting the four constants in both regions, experimental data may be well reproduced. Another simple approach, the back-shifted Fermi gas model was later proposed [11, 12, 13, 14] in order to account for shell effects. In this model, both the energy shift and the level density parameter a are considered as adjustable parameters, which allows to obtain a reasonable fit to the experimental level densities over a wider range of excitation energies. Afterwards, some phenomenological methods have been proposed to correctly describe the thermal damping of shell effects with increasing excitation energy (e.g. [15, 16, 17]). In those methods, the idea is to reproduce as well as possible the energy dependence of the level density parameter a taken from microscopic calculations, in order to give better absolute values of the nuclear level density.

However, most of the above-mentioned semiempirical approaches are based on various dras-

tic approximations, and their shortcomings at matching experiments are often overcome only by parameter adjustments. Therefore, the quality of the phenomenological prescriptions for a wide range of mass numbers can not be taken as a support for their accuracy outside the narrow regions of excitation energy ($\sim$ 5-15 MeV) and angular momentum ($\sim$ 0-5 $\hbar$) to which most of the experimental knowledge of level densities is confined. Numerical statistical calculations have also been developed to calculate a more realistic level density using the single-particle level scheme of the shell model [5, 18], and the BCS formalism has been included [19, 20] in order to account more properly for pairing effects. However, those microscopic calculations are still depending on the assumptions of the statistical model, namely the saddle-point approximation which is not very good at low energy. Moreover, the spin and parity distributions raise unsolved questions and call for improvement.

The advent of high speed computers has made possible to use methods of calculation which do not depend on closed formulae, such as the combinatorial method [21, 22, 23]. The level density is then calculated numerically by performing an exhaustive counting of the nuclear excited configurations. It yields an exact - at least in the independent-particle picture of the nucleus - level density, but is very time consuming and becomes intractable at high excitation energies or for large shell model spaces (i.e. for high-A nuclei). The pairing interaction may be included in the calculations by applying the BCS theory, but at the expense of a strongly increased computation time. More recently, combinatorial calculations have been carried out to estimate level densities with fixed exciton numbers [24], for use in preequilibrium models.

A second method of computing nuclear level densities directly from a set of single-particle states has been proposed by Williams [25], in order to avoid the direct enumeration and classification of states which renders the combinatorial method generally cumbersome. It is based on the repetitive use of recursion relations to expand the grand partition function, but it does not rely on the saddle-point approximation like the traditional statistical method. This so-called recursive method provides an exact calculation of level densities, but, compared with the combinatorial approach, it has the advantage of requiring far shorter computation time. It has been been extended in ref. [26] in order to describe the spin-parity distribution, and also to provide state densities with fixed particle-hole number. Unfortunately, it cannot treat residual interactions exactly, at least in its classical form, so that it is useful in the framework of a non-interacting Fermi gas model only. Spectral distribution methods [27, 28] (based on moment techniques to calculate averaged distributions of the Hamiltonian eigenvalues) have been used to provide level densities taking residual interactions into consideration. However, these methods are generally limited to a low-order expansion, which is not very accurate for large shell model spaces. Thus, for different reasons, both the combinatorial and the recursive methods are inappropriate to yield microscopic level densities including residual interactions in a reasonable computation time.

In this paper, we propose a Monte Carlo method as an alternative to the traditional combinatorial method. We calculate the level densities of spherical nuclei by means of a Monte Carlo simulation based on the Metropolis sampling scheme [29]. We show that this technique, initially devised for the simulation of molecular systems, can be successfully applied to the nuclear level

density problem. It yields an exact - save the statistical errors - level density within a short cpu time, whatever the mass number of the nucleus or the considered excitation energy. We also use this Monte Carlo method to calculate the spin and parity distributions of the excited levels. In this first attempt, we restrict ourselves to the case of spherical nuclei, but the method could be easily extended to deformed nuclei. A detailed description of the Monte Carlo method is given in Section 2. In Section 3, we check the reliability of this Monte Carlo procedure by comparing our results with those of a direct counting and with microscopic statistical calculations. Section 4 is devoted to the inclusion of pairing interaction in this model. Finally, we conclude in Section 5. The Monte Carlo implementation of the spin coupling and the statistical errors originating from the method are discussed in the Appendices. More detailed results and a comparison with experimental data are presented in a second paper [30].

2 The Monte Carlo method

As noted first by van Lier and Uhlenbeck [31], the nuclear level density problem in its simplest form (i.e. the uniform spacing model with one kind of particles) is equivalent to a well-known combinatorial problem in number theory, the partitioning of integers, first solved by Euler in the eighteenth century. Indeed, for a system of N fermions, the number $M = gU$ represents the number of quanta which are to be distributed among the N fermions, g and U being the single-particle state density and the excitation energy, respectively. Thus, the state density

$$\omega(U) = g \, p_N(M) \tag{1}$$

is proportional to the number $p_N(M)$ of partitions of the integer M into no more than N positive parts (see [32]). Note that an approximate solution for Euler's problem was derived by Hardy and Ramanujan in ref. [33], giving

$$p_N(M) \simeq \frac{\exp(\pi \sqrt{\frac{2}{3} M})}{\sqrt{48} M} \, , \tag{2}$$

when $N \geq M$ (i.e., when the excitation energy is not sufficient to excite a particle from the lowest orbit, which is clearly the case for an infinite model). This approximation is in fact equivalent to Bethe's formula

$$\omega(U) \simeq \frac{\exp(2\sqrt{aU})}{\sqrt{48} U} \, , \tag{3}$$

with the parameter $a = \frac{\pi^2}{6} g$. As investigated by Euler, the exact $p_N(M)$ can be calculated by means of the recursive relation [32]

$$p_N(M) = p_{N-1}(M) + p_N(M - N) \, . \tag{4}$$

It is instructive to notice that this relation is of the same class as Williams recursive relation [25] for the calculation of level densities in the uniform spacing model. However, the Williams

method is also applicable for a non-equidistant single-particle level scheme by expressing the single-particle energies as multiple of an energy unit (chosen approximately equal to the accuracy on the energies, e.g. 0.01 MeV). In this case, the level density problem comes to a more complex problem known in computer science as the subset-sum problem, for which the best algorithmic solution is a recursive one [34]. Unfortunately, as mentioned above, the recursive method can not incorporate residual interactions, so that recourse to a direct counting method cannot be avoided when treating pairing interaction. On the other hand, it is well known that a direct counting of all the excited nuclear levels is a very tedious task, almost impracticable on the currently available computers whenever one is interested in medium mass nuclei at intermediate energies. Moreover, a direct counting procedure cannot easily treat the residual interaction in nuclei because it is then exceedingly time-consuming. Thus it is natural to resort to a Monte Carlo technique in order to avoid this exhaustive counting of the excited levels. Furthermore, it is well known that Monte Carlo methods provide generally very efficient algorithms for solving combinatorial problems (e.g. combinatorial optimisation problems solved by simulated annealing [35, 36]). This is the main reason why we investigate the use of a Monte Carlo technique in the context of the nuclear level density problem, and this idea has been first explored in ref. [37]. This Monte Carlo method becomes essential if the residual interactions are taken into account, since the recursive method is intractable in this case. For simplicity, however, we consider the nucleus as a system of non-interacting fermions in this Section. This choice will allow a comparison with a direct counting in Section 3. The inclusion of the residual interactions is the subject of Section 4.

2.1   Principle of the Monte Carlo procedure

We present in this Section a Monte Carlo method based on the Metropolis sampling scheme which makes possible the determination of a combinatorial level density without direct counting. The Metropolis technique was devised for the simulation of molecular systems [29]; it has since been widely applied in statistical mechanics (e.g. to calculate thermal averages) [38, 39, 40]. We show here that it is convenient for describing nuclear level densities as well. Note that Monte Carlo simulations related to the level density problem have been performed in ref. [41] to obtain quantities of interest for the determination of the parity distribution. However, that work was done in the framework of the statistical model, which appears to be unable to treat correctly the parity dependence of the level density [42].

The Monte Carlo simulation is based on a random sampling of a very small fraction of the excited states in the considered range of excitation energy [43]. The resulting sample is assumed to be representative of the whole configuration space, in analogy with what is done when estimating a multi-dimensional integral by a Monte Carlo procedure (see e.g. [38]). Since the state density of a system of non-interacting fermions may be trivially expressed as

$$\omega(U, J, \pi) = \sum_C \delta(U - U_C) \ \delta_{J,J_C} \ \delta_{\pi,\pi_C} \ , \tag{5}$$

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i.e. as a multi-dimensional summation in a discrete space of configurations (each configuration C having an excitation energy U_C, spin J_C, and parity π_C), it can be efficiently obtained by a Monte Carlo sampling procedure. Note that each N-particle state is called here a configuration; it corresponds to the set of occupation numbers for all the single-particle states. (This is often called a combination in combinatorial methods terminology). It is clear that such a procedure cannot yield the whole ensemble of δ-spikes, but it is not important in practice, since only the average state density in energy bins is needed. Thus, the properties of the whole spectrum of excited states (i.e., energy, spin, parity, or other quantities) can be simply derived by extrapolating from the sample and applying the appropriate scale factor. This procedure provides an *exact* state density in the sense that it is independent of the grand-canonical statistical formalism (i.e., the energy and the number of neutrons or protons are not fixed only on average, which is a well-known source of errors). Of course, one has to keep in mind that the results are inherently affected by a statistical error.

A Monte Carlo estimator for the state density can be simply written as

$$\omega(U, J, \pi) \simeq S \, \omega_{\text{smp}}(U, J, \pi) \; , \tag{6}$$

where S is the scale factor (to be determined) and ω_{smp} stands for the state density in the Monte Carlo sample. One has

$$\omega_{\text{smp}}(U, J, \pi) = \sum_{i=1}^{N} \delta(U - U_i) \, \delta_{J,J_i} \, \delta_{\pi,\pi_i} \; , \tag{7}$$

where the C_i are randomly (uniformly) sampled configurations (of energy U_i, spin J_i and parity π_i) in the whole space, and N is the number of configurations in the Monte Carlo sample. The scale factor can be expressed as

$$S = (\sum_{C} 1)/N \; , \tag{8}$$

but it can not be calculated by this method, since the summation is prohibitively long in our configuration space ($\sum_C 1$ is intractable). It has to be determined by an independent method (see below).

Such an approach to the nuclear level density problem, introducing random excited configurations, may be quite justified. Indeed, the probability theory has already been applied with success in the statistical model to determine the asymptotic gaussian-shaped spin distribution and the parity distribution (see e.g. [3]). Furthermore, the nuclear level density problem may be seen as the problem of exploring a very large multidimensional space of configurations. A Monte Carlo simulation is recognized to be the best technique for solving this problem, and is in fact the only available one in many cases [38]. Note that, although the method is exact in principle, the resulting ω is inherently affected by a statistical error which scales like $1/\sqrt{N}$ (see Appendix A). The counterpart of this problem is that the accuracy of the results can be imposed by choosing an appropriate size N for the sample, and *do not depend* on the actual number of states in the considered energy range. (For instance, a rough estimate may be obtained within a very short computation time by sampling only a few configurations.) On the

contrary, when doing a direct counting of the states, the whole configuration space has to be explored, yielding an exact result within a computation time which can be prohibitively long. There is no other alternative. This fact constitutes the major advantage of a Monte Carlo procedure.

2.2 The Metropolis sampling scheme

It is clear that a simple random sampling of the states would be completely unefficient, since the state density $\omega(U, J, \pi)$ increases exponentially with excitation energy U. It is necessary in our simulation to hinder the random sampling of the highly excited configurations which are by far the most numerous, in order to achieve the same level of accuracy over the whole considered energy range. Therefore, we have to apply an importance sampling method (see e.g. [38]). Let us introduce a (discrete) probability distribution $P(C)$. The Monte Carlo evaluation of $\omega(U, J, \pi)$ becomes

$$\omega(U, J, \pi) \simeq \frac{1}{N} \cdot \sum_{i=1}^{N} \frac{\delta(U - U_i) \, \delta_{J,J_i} \, \delta_{\pi,\pi_i}}{P(C_i)} \ , \tag{9}$$

whenever each C_i is randomly sampled with a probability $P(C_i)$. The problem is that the probabilities $P(C_i)$ cannot be simulated (neither calculated) because it is impossible to perform the normalization in our configuration space. The Metropolis method provides a solution for this problem by only referring to ratios of probabilities, and makes thus an importance sampling procedure practicable.

The Metropolis sampling scheme allows to produce any random variable in many dimensions with a given probability distribution. It only requires the ability to calculate a weight function (proportional to the probability) for a given value of the integration variable. Let us define a weight function $W(C)$ that represents in our problem the *relative* (unnormalized) sampling probability of the configuration C, i.e., $W(C) \propto P(C)$. At this point, $W(C)$ is arbitrary, but we will show how to define it properly in the following. The Metropolis method is based on a guided random walk which proceeds through configuration space according to a given matrix of transition probabilities $\mathbf{p}$. Each element $p(C_a \to C_b)$ of this matrix corresponds to the probability of performing a step from the state (or configuration) a to the state b. The Metropolis method prescribes the choice of this stochastic matrix $\mathbf{p}$ in order to obtain a random walk with a limit distribution (i.e., the distribution of the frequencies with which each state occurs when letting the random walk run to infinity) equal to a given $P(C)$:

$$p(C_a \to C_b) = \begin{cases} q(C_a \to C_b) & \text{if } W(C_b) \geq W(C_a) \ , \\ q(C_a \to C_b) \cdot \dfrac{W(C_b)}{W(C_a)} & \text{if } W(C_b) < W(C_a) \ , \end{cases} \tag{10}$$

where $\mathbf{q}$ is the so-called underlying matrix of the random walk, and will be defined below. In order to completely define the random walk process, the diagonal elements of the stochastic

matrix must be taken as

$$p(C_a \rightarrow C_a) = 1 - \sum_{b \neq a} p(C_a \rightarrow C_b) \ . \tag{11}$$

This Metropolis prescription has been proved to be rigorous for a discrete space [38], which is just the case for our nuclear configuration space. Indeed, it is easy to check, using equation (10), that the detailed balance $P(C_a) \, p(C_a \rightarrow C_b) = P(C_b) \, p(C_b \rightarrow C_a)$ is verified provided that $\mathbf{q}$ is a symmetric matrix. This clearly implies that, conditionally on the ergodicity of the random walk, the correct limit distribution is reached. As already mentioned, expression (10) only refers to the weight function $W(C)$, and is thus tractable.

From the definition of the stochastic matrix $\mathbf{p}$, it appears that each step (from state a to b) can be decomposed into two stages. The first one, corresponding to the stochastic matrix $\mathbf{q}$, consists in the random choice of a trial move. Thus, $q(C_a \rightarrow C_b)$ stands for the probability to perform a trial move from state a to b. Note that the Metropolis method requires $\mathbf{q}$ to be a symmetric matrix, so that the reverse move from state b to a has the same probability as the forward move. The next stage is the decision to either accept or reject this trial move, the probability of accepting or rejecting a trial move depending on the given weight function $W(C)$, as shown in (10). If the trial move is rejected, the system stays in the same state, that is $b = a$.

Now, forming a long enough random walk following this procedure, we have a new Monte Carlo estimator for the state density

$$\omega(U, J, \pi) \simeq S \ \sum_{i=1}^{N} \frac{\delta(U - U_i) \ \delta_{J,J_i} \ \delta_{\pi,\pi_i}}{W(C_i)} \ , \tag{12}$$

where the C_i are the random configurations along the random walk of length N. Here, the scale factor is defined by

$$S = \left(\sum_C W(C) \right) /N \ . \tag{13}$$

The second factor in the right-hand side of equation (12) represents the (corrected) state density in the Monte Carlo sample, i.e., $\omega_{\text{smp}}(U, J, \pi)$. Thus, each sampled configuration C_i is given an importance $1/W(C_i)$ that is inversely proportional to its sampling probability $P(C_i)$.

2.3 Implementation of the Monte Carlo calculation

In our calculation, each state belonging to the random walk corresponds to a configuration C, i.e., it is associated with a set of occupation numbers $\{n_k^\nu(C); n_k^\tau(C)\}$ for all the neutron and proton single-particle states. Thus, the successive configurations are chosen randomly (according to the stochastic matrix $\mathbf{p}$) as follows. First, one selects a nucleon at random (either a neutron with probability N/A or a proton with probability Z/A) and moves it to a randomly chosen available single-particle state. This generates a new configuration. (This single-particle trial move corresponds to our definition for the underlying matrix of the random

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walk $\mathbf{q}$, and is the most common choice for the elementary move. This sampling procedure is shown in ref. [44] to be generally more efficient than collective moves, with several particles moved simultaneously.) Then, one accepts or rejects this single-particle trial move according to equation (10). This acceptance criteria will thus depend on $W(C)$, which will be in general a function of U_C, J_C, and π_C. In our calculation, an energy dependence has proven to be sufficient, so that we choose $W(C)$ as a function of U_C only. This weight function is arbitrary in principle: different choices give the same result for an infinitely long random walk. However, a judicious choice makes the method much more efficient than the simplest choice $W(C) = 1$. Indeed, we have to compensate for the rapid increase of the number of states with energy by selecting a correspondingly decreasing weight function. An appropriate choice would be to take $W(C)$ proportional to the inverse of a Bethe-type law,

$$W(C) = (a\ U_C)^{5/4}\ \exp\left[-2\ (a\ U_C)^{1/2}\right]\ , \tag{14}$$

in which the parameter a is adjusted to ensure a more or less uniform distribution of the sampled states in the considered energy interval. We took this definition of $W(C)$ in our previous work (see [37]), for simplicity. In this paper, we prefer another definition based on a recursive model calculation. This will be discussed later on.

Let us consider now the energy, spin, and parity assignment for each randomly sampled configuration. The excitation energy U_C of each configuration C (when assuming a system of non-interacting fermions) is simply given by the sum of the energies of all the occupied single-particle states

$$U_C = \sum_k \epsilon_k^\nu \cdot n_k^\nu(C) + \sum_k \epsilon_k^\pi \cdot n_k^\pi(C)\ -\ E_0\ , \tag{15}$$

where the $n_k^{\nu,\pi}(C)$ are the occupation numbers for the configuration C, and the $\epsilon_k^{\nu,\pi}$ are the single-particle energies for neutrons and protons. The ground state energy is noted as E_0. It is clear that, with our procedure, each excited level will be sampled with a probability proportional to its statistical weight, as expected. Suppose for instance that we are interested in the level corresponding to a $(1d_{5/2})^3$ configuration, having a degeneracy $d = \binom{6}{3} = 20$. It will obviously be sampled with a probability proportional to the number of possible arrangements of 3 particles into 6 orbits, that is to d. The possible inclusion of pairing energy using BCS theory (removing this degeneracy) will be examined below.

The spin J_C of each configuration C is chosen randomly among all the possible spins of its associated excited level; we choose the sampling probabilities of all the spins according to their respective degeneracies. In order to achieve this random choice, we proceed as follows. First, we determine the total spin of identical nucleons in each subshell. In order to account for the Pauli principle, we use the so-called Mayer-Jensen table [22, 45] which yields the number of times each spin occurs. Thus, the spin is chosen at random with a probability distribution determined according to this table, as explained in Appendix B. Then, the spins of the different subshells are coupled randomly, for either type of nucleons separately. For this purpose, we use the relation

$$J = j_1 + j_2 - \min(d_1, d_2) \tag{16}$$

for the coupling of two spins (j_1 and j_2) to a total spin J, where d_1 and d_2 are (discrete) random variables uniformly distributed in $[0,2j_1]$ and $[0,2j_2]$ respectively. It can be shown (see Appendix B) that this relation yields a total spin J obeying the usual coupling rule of angular momentum for independent particles, with adequate weights (i.e., the sampling probability of each spin is proportional to its degeneracy). Thus, relation (16) is applied recursively in order to couple the spins of all the subshells. Finally, the total neutron and proton spins are coupled at random, also using equation (16), to give the resulting spin of the configuration J_C. Note that, when doing a direct counting of the levels, the whole ensemble of possible spins (for each excited level) has to be enumerated. On the contrary, the Monte Carlo determination of the spin distribution is far simpler: one has just to choose one of these spins with the appropriate probability, which is much less time-consuming.

The parity of the sampled configurations is also easily obtained by combining the parities of all the occupied single-particle states. Thus, the resulting parity π_C of a configuration C is given by

$$\pi_C = \prod_k [\pi_k^\nu]^{n_k^\nu(C)} \prod_k [\pi_k^\pi]^{n_k^\pi(C)} , \tag{17}$$

where the $\pi_k^{\nu,\pi}$ are the single-particle state parities.

Finally, one has to determine the scale factor S needed to obtain an *absolute* state density. To this end, we calculate the total number of states $N_{\rm rec}$ up to our maximum energy $U_{\rm max}$ (the upper limit of the energy interval of interest) by means of the Williams recursive method [25]:

$$N_{\rm rec} = \int_0^{U_{\rm max}} \omega_{\rm rec}(U) \; {\rm d}U . \tag{18}$$

Thus, we have a constraint on the Monte Carlo cumulative state density at energy $U_{\rm max}$,

$$N(U_{\rm max}) = \int_0^{U_{\rm max}} \sum_J \sum_\pi \omega(U, J, \pi) \; {\rm d}U = N_{\rm rec} , \tag{19}$$

which gives obviously for the scale factor $S = N_{\rm rec}/N$. This simple recursive method can neither yield the spin-parity distribution, nor take into account a residual interaction. However, we just need it to normalize our Monte Carlo sample state density $\omega_{\rm smp}(U, J, \pi)$. Moreover, as it provides the whole state density curve as a function of the energy, $\omega_{\rm rec}(U)$, we can use it in order to define our weight function as explained in Appendix A. This choice for $W(C)$ ensures a more or less uniform distribution of the sampled states in the considered energy interval. As a consequence, the resulting state density $\omega(U, J, \pi)$ is more or less equally accurate in the whole energy interval. Note that we reject the sampling of excited states above the upper limit $U_{\rm max}$ by putting $W(C) = 0$ for $U_C > U_{\rm max}$. This recursive calculation of the state density takes a very short computation time.

For illustrative purposes, we have calculated the Monte Carlo level density of ^{56}Fe up to an excitation energy of 30 MeV, using the realistic set of single-particle levels derived from a spherical Hartree-Fock calculation based on a Skyrme interaction [46]. In order to obtain a reasonable accuracy, the size of the sample N (which crucially determines the computation

time) is adopted equal to 10^6. Figure 1 shows the derived cumulative state densities (i.e. the number of states up to a given energy U). The solid line represents the total cumulative state density (with both parities), while the positive- and negative-parity cumulative state densities are represented by dashed and dash-dotted lines, respectively. The curves show an overall behaviour in agreement with the statistical results, i.e. an asymptotic parabolic shape versus energy (in logarithmic scale). However, superimposed small-scale oscillations are pronounced at low energies, and disappear only at higher excitation. We also notice that the classical assumption of equipartition of both parities [3] is only valid above ~ 15 MeV. Note that we obtain a high degeneracy for the ground state because of the neglect of residual interactions. Of course, this degeneracy would be removed if residual interactions were included in our model (see Section 4). For information, we also plot in Figure 1 the cumulative number of sampled states along the Monte Carlo simulation. It is evident that the excited states have been sampled approximately uniformly over the whole energy interval [0–30 MeV], as expected, so that the resulting accuracy is roughly constant (see Appendix A).

3 Results

We will show in this Section that the Monte Carlo procedure is very efficient for calculating an exact - at least in principle - level density with spin and parity dependence, whatever the mass number of the nucleus or the considered excitation energy. Other quantities, such as the fixed particle-hole number level densities, could also be obtained by this method. In this respect, the Monte Carlo method must be considered as a way to implement the calculation of a combinatorial level density, replacing a direct counting procedure when it is unfeasible (for large shell model spaces). However, a direct counting of the levels can be helpful when the number of excited levels is directly computable, in which case a Monte Carlo sampling would introduce undesirable statistical errors.

In ref. [37], we reported on the Monte Carlo derived level density of ^{56}Fe, ^{208}Pb, and ^{140}La. We chose the same size for the sample, i.e., $N = 10^6$, which gave essentially the same accuracy in the three cases although the fraction of the whole set of excited states that is actually sampled is about 3×10^{-4} for ^{56}Fe, 10^{-7} for ^{208}Pb, and only about 2×10^{-9} for ^{140}La. With such a choice, it is remarkable that the Monte Carlo simulation takes about the same computation time for the three nuclei, although their mass numbers are very different. Some other cases can be found in ref. [47]. In the following, we will limit ourselves to check the method by comparing with other traditional methods for calculating level densities. New results will be discussed in greater details in ref. [30].

3.1 Comparison with a direct counting

In order to verify the reliability of our Monte Carlo procedure, we have performed calculations of the level density and spin-parity distribution via a direct counting of the levels (see ref. [48]). We

have considered in particular the case of ^{56}Fe up to 30 MeV, neglecting the pairing interaction and using the single-particle levels from ref. [46]. Note that a combinatorial calculation at such excitation energies is still feasible in this mass number region, although at the cost of an impressive cpu time. The total state density derived with the Monte Carlo method could hardly be distinguished on Figure 1 from the direct counting [48], so that we did not plot the latter. In fact, the tiny difference is simply due to the statistical noise (which can be made arbitrarily small by increasing N). Of course, the recursive method also gives identical results, but, nevertheless, it is impracticable when considering residual interactions.

Let us turn now to the spin dependence of the ^{56}Fe level density. In Figure 2, we plot the spin distribution of the levels in the energy interval [20–21 MeV] derived by the Monte Carlo method, along with the direct counting calculation [48]. The square symbols and the solid line represent, respectively, the result of the Monte Carlo method and the direct counting. The Monte Carlo spin distribution is obtained by putting $W(C) = 1$ from $U = 0$ to the upper limit $U = 21$ MeV. Thereby, the states with high excitation energy are sampled preferentially, and the accuracy on the spin distribution is increased. The adopted sample size is $N = 50 \times 10^6$, in order to get very good statistics (to have negligible statistical errors). Of course, such an accuracy might be unnecessary for practical applications, but our intention here is just to show that the Monte Carlo result is asymptotically exact. Indeed, both Monte Carlo and direct counting calculations are in very good agreement, showing the validity of the random spin coupling procedure explained in Section 2. Note that, in this high energy domain, the number of excited levels is as high as 2×10^6, so that the spin distribution is expected to be consistent with the asymptotic distribution of the statistical model (see Figure 3). The positive- and negative-parity spin distributions obtained by the Monte Carlo method are also shown in Figure 2. It appears that, in spite of this large number of levels, the parity equipartition is not achieved yet in the considered energy interval, illustrating the need for an appropriate treatment of parity (see [42]).

In the conventional statistical model, the dependence of the state density upon the angular momentum projection M has the gaussian form [3, 4]

$$\omega(U, M) = \omega(U)\frac{\exp(-M^2/2\sigma^2)}{\sqrt{2\pi\sigma^2}} \,, \tag{20}$$

where σ^2 is the spin cut-off parameter, and $\omega(U)$ stands for the total state density. The resulting spin-dependent level density can be written as [2]

$$
\begin{aligned}
\rho(U, J) &= \omega(U, M = J) - \omega(U, M = J + 1) \\
&\simeq -\left[\frac{\mathrm{d}}{\mathrm{d}M}\,\omega(U, M)\right]_{M=J+1/2} \\
&\simeq \frac{2J + 1}{2(2\pi)^{1/2}\sigma^3}\exp\left[-\frac{(J + 1/2)^2}{2\sigma^2}\right]\omega(U) \,,
\end{aligned}
\tag{21}
$$

where J denotes the total angular momentum of the levels at excitation energy U.

We check in Figure 3 that our Monte Carlo derived spin distribution for ^{56}Fe in [8–10 MeV] looks similar to the gaussian-shaped asymptotic distribution. We plot the M-distribution of the excited states (i.e., $\omega(U, M)$ as a function of M). The agreement with the gaussian form (20) is evident, as expected given the excitation energy. We estimate an effective spin cut-off parameter σ^2 by calculating the variance of this M-distribution. This yields the value $\sigma^2 \simeq 18.8$, corresponding to a maximum in the J-distribution at a spin around $\sigma \simeq 4$. The gaussian distribution with this adopted value for σ^2 is plotted. Figure 3 also shows the corresponding J-distribution of the excited levels simulated by Monte Carlo, as well as the asymptotic distribution (21) obtained with the same value of σ^2. It proves that one can be confident in the asymptotic result if one is concerned with an energy interval containing a sufficiently large number of levels. Indeed, the number of levels amounts to 8×10^3 in our case. However, when considering an interval containing fewer levels, the assumption of a gaussian distribution becomes very poor (see e.g. [37, 47]). It is interesting to note that the discrepancy between the curves is more pronounced when looking at the J-distribution, showing that the latter is more sensitive to deviations from asymptotic results.

Finally, the evolution of the parity distribution of the excited levels in ^{56}Fe as a function of energy (up to 30 MeV) is shown in Figure 4. We plot, as a function of U, the cumulative parity asymmetry defined by

$$A = \frac{N^+(U) - N^-(U)}{N^+(U) + N^-(U)} \,, \tag{22}$$

with $N^\pm(U) = \int^U \omega^\pm(U) \, \mathrm{d}U$. The dotted line corresponds to the Monte Carlo results, whereas the solid line is calculated by a direct counting of the levels [48]. Once more, both curves are almost indistinguishable. This proves that the Monte Carlo method is a powerful alternative to the traditional combinatorial method; it reproduces the parity-asymmetry curve derived by direct counting within an asymptotically small statistical error and with a huge gain of cpu time. Note that the parity equipartition, generally assumed to be achieved at low energies, is only reached above ~ 15MeV. This point is examined in greater detail in ref. [42].

3.2   Comparison with a microscopic statistical model

In order to illustrate the reliability of our Monte Carlo procedure, we have also compared our results with the predictions of a numerical statistical model. This model, based on the traditional methods of statistical mechanics, takes into account the shell effects by using a realistic discrete single-particle spectrum (see e.g. [4]). The total energy E, the number of neutrons N and protons Z, and the entropy S are determined from the single-particle energies ϵ_k^ν (for neutrons) and ϵ_k^π (for protons) by the relations

$$E = -\frac{\partial \Omega}{\partial \beta} \,, \tag{23}$$

$$N = \frac{\partial \Omega}{\partial \alpha_N} \,, \tag{24}$$

$$Z = \frac{\partial \Omega}{\partial \alpha_Z} \, , \tag{25}$$

$$S = \Omega - \alpha_N N - \alpha_Z Z + \beta E \, , \tag{26}$$

with

$$\Omega \equiv \ln Z = \sum_k \ln[1 + \exp(\alpha_N - \beta \epsilon_k^\nu)] + \sum_k \ln[1 + \exp(\alpha_Z - \beta \epsilon_k^\pi)] \, , \tag{27}$$

where Z is the partition function, and α_N, α_Z, $\beta = 1/t$ are the Lagrange multipliers related, respectively, to the number of neutrons, the number of protons, and the total energy. One also defines the quantity D as the 3×3 determinant of the second derivatives of Ω with respect to α_N, α_Z, and β, evaluated at the saddle point. All these quantities can be calculated numerically, and the resulting state density for a two-component system is given by

$$\omega(E, N, Z) = \frac{\exp S}{(2\pi)^{3/2} D^{1/2}} \, . \tag{28}$$

These calculations were performed using the statistical method from ref. [49], based on a realistic spectrum of single-particle levels from ref. [46], neglecting the pairing interaction.

In Figure 5a, we show the state density for ^{56}Fe calculated by this statistical method for comparison with the combinatorial (Monte Carlo) result. The solid line represents the state density obtained with our Monte Carlo method, plotted in bins of 100 keV, while the dashed line corresponds to the statistical model calculation. Both curves were calculated using the same set of single-particle levels. Note that the noisy behaviour of the Monte Carlo state density at low energies comes from the fact that a lot of bins are devoid of levels. Of course, the curve could be smoothed by increasing the bin width, but the oscillations (due to the discrete structure of the single-particle spectrum) would then be smeared out. The agreement between statistical and combinatorial state densities is reasonable, even if those oscillations disappear completely in the statistical formalism. The statistical state density can thus be viewed as an average of the combinatorial state density, which is obviously a consequence of the grand-canonical approach (the energy is only fixed on average). Note that the statistical curve looks higher than the averaged combinatorial curve, but this is simply due to the logarithmic scale. It has to be stressed that the discrepancies between both methods (ranging up to one order of magnitude) might be significant e.g. when calculating reaction cross sections with statistical or Monte Carlo level densities. We also consider the case of a heavier odd-odd nucleus in Figure 5b. We compare the combinatorial (Monte Carlo) and statistical state densities for ^{140}La (assumed to be approximately spherical, and without pairing). The solid and the dashed line correspond, respectively, the Monte Carlo and the statistical state density. The latter curve also appears as an averaged combinatorial state density, even if a little systematic error seems to be present. A small statistical noise is still visible in the Monte Carlo state density, related to the choice of the sample size $N = 10^6$.

Let us consider now the spin distribution in this microscopic statistical model, and in particular the evolution of the spin cut-off parameter with energy. Within the framework of the

statistical model, one can generalize the formalism by adding a supplementary Lagrange multiplier γ related to the angular momentum projection M (see [4]). It can be shown that, except for extremely large values of M, the Lagrange multiplier γ is sufficiently small to obtain a good approximation by expanding the statistical expressions in powers of γ, and by keeping the terms up to γ^2 only. The thermodynamic quantities of interest can be written in terms of γ as in equations (23)-(26). By eliminating γ, one gets an expression for the M-dependent state density similar to equation (20),

$$\omega(E, N, Z, M) = \omega(E, N, Z)\frac{\exp(-M^2/2\sigma^2)}{\sqrt{2\pi\sigma^2}} \; , \tag{29}$$

where $\omega(E, N, Z)$ is the total state density defined in equation (28). The spin cut-off parameter which determines the width of the M-distribution is given by the expression:

$$\sigma^2 = \frac{1}{4}\sum_k (m_k^\nu)^2 \mathrm{sech}^2\frac{1}{2}(\beta\epsilon_k^\nu - \alpha_N) + \frac{1}{4}\sum_k (m_k^\pi)^2 \mathrm{sech}^2\frac{1}{2}(\beta\epsilon_k^\pi - \alpha_Z) \; , \tag{30}$$

where m_k^ν and m_k^π are the single-particle magnetic quantum numbers for neutrons and protons, respectively. The resulting spin-dependent level density $\rho(E, N, Z, J)$ can be expressed as in equation (21).

In Figure 6, we compare the effective spin cut-off parameters of three nuclei (^{120}Sn, ^{162}Dy, and ^{208}Pb) derived from our combinatorial (Monte Carlo) method and from a numerical statistical model (ref. [49, 50]). Both predictions make use of the same Woods-Saxon single-particle level scheme. The Monte Carlo spin cut-off is derived by calculating the variance of the M-distribution, as previously. As can be seen, the Monte Carlo method leads to a rather good prediction of the energy-dependent effective spin cut-off parameter, showing that one can be confident in the method. Note that, even if this agreement for σ^2 is very satisfying, the statistical assumption of a gaussian distribution is not always justified (see [37, 47]), so that our Monte Carlo procedure can become essential in some cases.

4   Pairing interaction

In our previous work [37], we restricted ourselves to the Monte Carlo evaluation of the level density without the inclusion of pairing force. In this Section, we explore the possibility to account for the pairing interaction in the Monte Carlo method. The pairing interaction is usually taken into account in combinatorial calculations by use of the BCS theory (see ref. [22, 24]). For example, Hillman and Grover [22] corrected their combinatorially calculated level density for pairing forces by solving the BCS equations (at zero temperature) for each excited configuration. They used two so-called "interacting odometers" to scan the nuclear configurations systematically, one for the unpaired nucleon configurations (determining the spin distribution), the other one for the pair configurations. They extended the "blocking" method developed in ref. [51] for treating odd-A nuclei (with one unpaired nucleon) to the case of configurations

containing more than one unpaired nucleon: all orbital pairs containing unpaired nucleons are blocked (i.e., made unavailable for pair diffusion by being omitted from the BCS calculation). In their model, the total energy of a (proton or neutron) configuration C is given by

$$E_C = {\sum_k}' \, \epsilon_k + {\sum_k}'' \, 2\epsilon_k v_{k,C}^2 - \Delta_C^2/G \;, \tag{31}$$

where G is the pairing strength parameter, and $v_{k,C}^2$ is calculated from

$$v_{k,C}^2 = \frac{1}{2}\left\{ 1 - \frac{\epsilon_k - \lambda_C}{[(\epsilon_k - \lambda_C)^2 + \Delta_C^2]^{1/2}} \right\} \;, \tag{32}$$

Δ_C and λ_C being obtained by solving the pair of BCS equations

$${\sum_k}'' \, 2v_{k,C}^2 = \eta_C \;, \tag{33}$$

$${\sum_k}'' \, [(\epsilon_k - \lambda_C)^2 + \Delta_C^2]^{-1/2} = 2/G \;. \tag{34}$$

Here, Δ_C and λ_C are the gap parameter and Fermi energy, respectively, while η_C stands for the number of paired nucleons. The summation $\sum'$ is made over orbitals containing unpaired nucleons, while $\sum''$ is made over orbital pairs in which there is not an unpaired nucleon. Note that, as the excitation energy increases, more and more orbital pairs are blocked, so that only the trivial solution $\Delta = 0$ can exist in general above a certain energy. This behaviour is in qualitative agreement with the result of the temperature-dependent BCS theory [19].

However, the model of Hillman and Grover has an inherent drawback related to the configurations involving promoted pairs. Due to its variational nature, the BCS method cannot treat a general configuration of pairs, but only yields the energy of the particular configuration where the pairs are all placed in the lowest available (unblocked) orbitals. They accounted for this problem by adding to the BCS energy the difference in single-particle energy of that particular configuration of pairs and the one under consideration. They claimed that, even if this is clearly a rough approximation, the resulting error is not very serious because the fraction of levels with pair excitation is small.

The combinatorial model of Herman and Reffo [24] is slightly different, although the pairing interaction is also included by applying the BCS theory to each configuration. As they were interested in estimating a level density with fixed exciton numbers, they simply neglected the excitations involving promoted pairs. All the excited particles are taken as noninteracting excitons, and the orbitals in which they are placed are excluded from the BCS consideration, even if two particles occupy time-reversed orbitals. They also justified this approximation by arguing that the number of such configurations involving promoted pairs is very small.

In conclusion, it is our opinion that this problem of promoted pairs is due to the *hybrid* character of those methods. Indeed, BCS is inherently a statistical theory, and is therefore incompatible with any combinatorial procedure for estimating the level density. In fact, only

a kind of "combinatorial" treatment of the pairing interaction would give a consistent solution to the above problem. This is our purpose in ref. [52], where we propose a quantum Monte Carlo method to treat exactly the pairing force in nuclei. This method in its present status is, however, limited to the properties of the ground state, and is not directly applicable to the level density problem. Thus, in this paper, we have to limit ourselves to an approximate inclusion of pairing by use of the standard BCS theory, close to what is done in ref. [24], and we show it is feasible at essentially no cpu cost.

For each sampled excited configuration, we solve the BCS equations in order to obtain its pairing energy P_C. We also use the so-called blocking method [22, 51], that is the orbits occupied by unpaired nucleons are blocked (i.e., unavailable for pair diffusion). However, we treat the problem of the promoted pairs in a slightly different way: first, the number of unpaired nucleons occupying the Fermi level is taken equal to the seniority s derived from our random spin coupling algorithm, as explained in Appendix B. This will ensure that the spin attribution of the low-lying levels is coherent with the single-particle level scheme. Second, all the excited particles (and created holes) on the other levels are taken as noninteracting excitons, even if two particles (or holes) occupy time-reversed orbitals, in analogy with what is done in ref. [24]. We think that this is the simplest approximate prescription to properly construct the first excited states, while neglecting excitations involving promoted pairs at higher energies. Thus, the energy U_C of each sampled configuration is corrected for pairing and replaced by $U_C - P_C$ in equation (12), when computing the Monte Carlo state density:

$$\omega_P(U, J, \pi) \simeq S \sum_{i=1}^{N} \frac{\delta(U - U_i + P_i)\, \delta_{J,J_i}\, \delta_{\pi,\pi_i}}{W(C_i)} \;, \tag{35}$$

where P_i stands for the pairing energy of the configuration C_i (that is the sum of the pairing energies for neutrons and protons). Note that the energy used to calculate the weight function (see Appendix A) does not include this pairing term, so that the state density without pairing can also be computed at the same time. This state density is useful since it allows to perform the normalization according to ω_{rec}, which do not incorporate pairing energy, as already mentioned. In fact, the Monte Carlo simulation proceeds as if there was no pairing (the weight function is inversely proportional to ω_{rec}), and then the actual sampling of the configurations corrects for the effect of pairing.

In order to illustrate the effect of pairing, we have considered the isobars ^{142}Nd (even-even) and ^{142}Pr (odd-odd). For both nuclei, we use the spherical single-particle level scheme resulting from a Hartree-Fock + BCS calculation from ref. [46]. We solve the BCS equations for all the excited configurations with the values for the pairing strength parameters $G_n = 2.25/N^{0.7}$ MeV (for neutrons) and $G_p = 2.00/Z^{0.7}$ MeV (for protons) derived in ref. [46] for the ground state. In Figure 7, we plot the cumulative total state density including pairing effects derived with our Monte Carlo method for both ^{142}Nd (solid line) and ^{142}Pr (dash-dotted line), as a function of the excitation energy U. The effect of deformation is neglected here. The dashed and the dotted lines represent the cumulative state density for both nuclei in the absence of pairing. The latter curves clearly illustrate the existence of shell effects: as ^{142}Nd is situated at a neutron shell

closure, its level density is lower than that of the neighbour nucleus ^{142}Pr. In fact, given the similarity between the corresponding single-particle level schemes, this can be simply described as a Rosenzweig effect [53], resulting in a shell-correction shift in the energy scale. In addition, one can see in Figure 7 that, for both nuclei, the pairing force is responsible for a shift of the level density curve to the right, according to the classical phenomenological models (see e.g. [22]). Roughly speaking, this shift corresponds to the condensation energy of the ground state due to pairing. Therefore it is clear that, due to the even-even character of ^{142}Nd, its level density has to be shifted more than that of ^{142}Pr. (The condensation energy is found to be about 4.6 MeV for ^{142}Nd, and 3.3 MeV for ^{142}Pr.) The difference between both shifts is approximately equal to $\Delta_n + \Delta_p$, with Δ_n and Δ_p being respectively the gap parameter for neutrons and protons in ^{142}Nd. The Monte Carlo method is, of course, more accurate than a simple phenomenological model since it yields a shift varying with energy, and thus provides a supposedly more realistic level density.

Note that the extra amount of cpu time needed for the inclusion of pairing in our Monte Carlo procedure was found to be only about 30-40%. This fact seems surprising at first glance, since it is well known that a combinatorial computation becomes in general extremely time-consuming when treating residual interactions. It originates from the fact that only about 1% of the Metropolis trial moves are accepted on average along our random walk, so that the extra cpu time needed to compute the pairing energy (by solving BCS equations) only concerns about 1% of the configurations. Accordingly, the energy of the remaining (99%) configurations does not need to be calculated, allowing a significant gain of computing time. The latter configurations are necessary, however, to associate the appropriate statistical weights to the former 1% configurations that are effectively sampled.

Therefore, we think that a Monte Carlo evaluation of the level density with inclusion of pairing is very promising. If the pairing force could be accounted for in a consistent way (i.e., without the use of BCS theory), it would be the only available method for solving exactly this problem. It would not depend on the grand-canonical statistical formalism (finite-temperature BCS equations [19]) and its associated difficulties, such as the spurious phenomenon of a sharp superfluid-normal phase transition in nuclei [54]. The exact solution of this problem via a Monte Carlo procedure is the subject of a future work.

5   Conclusion

The Monte Carlo method is shown to be a reliable technique for calculating nuclear level densities with a sufficient accuracy within computation times that are much shorter than those demanded by traditional combinatorial methods (i.e., a direct counting). Also, owing to its rapidity, this method makes possible the estimate of the shell-model uncertainties (i.e., those associated with the single-particle level scheme). In the absence of residual interactions, however, the recursive method is exact as well and requires approximately the same amount of computation time. In any case, it is necessary to calculate the Monte Carlo scale factor by the

recursive method. Thus the Monte Carlo method really becomes a powerful tool when studying nuclear level densities with pairing interactions, as explored in Section 4. It would even be possible to include neutron-proton interactions in this method, which cannot be considered by any other method.

The Monte Carlo approach also turns out to be worthwhile to predict the excited levels spin and parity distributions. Considering the crude approximations made to obtain those distributions in the framework of the statistical model, the proposed method is an interesting alternative to the usual statistical methods used in nuclear reaction calculations. Moreover, the technique outlined in this paper could be extended to the case of deformed nuclei. More detailed calculations and a confrontation with experimental data are presented in a subsequent article [30].

Acknowledgments

Appendices

A   Statistical errors

Due to the principle of the Monte Carlo method (i.e., the sampling of a finite number of configurations), it is clear that a statistical noise is superimposed on the derived total state density and the spin-parity distribution. We will only consider here the case of the total state density, but the same reasoning also applies to the calculation of the statistical error on other quantities.

The continued evolution of the random walk yields successive configurations C that are distributed according to the weight function $W(C)$. This distribution is then sampled by repeated application of the stochastic process $p(C_i \rightarrow C_{i+1})$ defined in equation (10). The resulting Monte Carlo estimator for the total state density is thus given by

$$
\begin{aligned}
\omega(U) &= \left(\sum_C W(C) \right) \mathrm{E} \left[\frac{\delta(U - U_C)}{W(C)} \right]_{P(C)} , \\
&\simeq S \sum_{i=1}^{N} \frac{\delta(U - U_{C_i})}{W(C_i)} ,
\end{aligned}
\tag{36}
$$

where $S = \sum_C W(C)/N$ is the scale factor, and E[ ] means the expectation value for a random sampling of the configurations C according to the probability distribution $P(C) \propto W(C)$.

As explained in Section 2.2, the idea of the importance sampling procedure is to achieve a more or less uniform sampling in the considered energy range. Let us consider an energy bin of width ΔU, situated at an excitation energy U, containing a non-zero number of states. (If the bin is devoid of states, it must simply be excluded from the following considerations.) Let us call $\{\bar{C}\}$ the ensemble of configurations belonging to this bin (i.e., for which $U \leq U_{\bar{C}} \leq U + \Delta U$), and let us give them the same weight $\bar{W}(U)$ for simplicity. Assuming that the state density is constant inside this bin and equal to $\bar{\omega}(U)$, the weight of that bin is thus approximately $\bar{W}(U)\bar{\omega}(U)\Delta U$. The condition of a uniform sampling imposes thus that

$$\bar{W}(U)\bar{\omega}(U)\Delta U / \sum_C W(C) \simeq \Delta U/U_{\text{max}} \ , \tag{37}$$

where U_{max} is the upper limit of the considered energy interval. In practice, since $\bar{\omega}(U)$ is unknown, it is replaced by the derived state density from the recursive method. Equation (37) corresponds to our definition of the weight function $W(C)$.

According to equ. (36), the estimator for the number of states in that bin is obviously

$$\begin{aligned}
\mathcal{N}(U) &= S \sum_{i=1}^{N} \frac{\Theta(U_{C_i} - U)\Theta(U + \Delta U - U_{C_i})}{W(C_i)} \ , \\
&= \left(S/\bar{W}(U)\right) \sum_{i=1}^{N} \Theta(U_{C_i} - U)\Theta(U + \Delta U - U_{C_i}) \ , \tag{38}
\end{aligned}$$

where $\Theta(x)$ stands for the Heaviside step function. By integrating (36) between U and $U + \Delta U$, the expectation value of $\mathcal{N}(U)$ is trivially given by

$$\mathrm{E}[\mathcal{N}(U)] = \int_{U}^{U+\Delta U} \omega(U)\mathrm{d}U = \bar{\omega}(U)\Delta U \ . \tag{39}$$

In order to estimate the statistical noise on $\mathcal{N}(U)$, let us define first the probability of choosing a random configuration in this bin as $\mathcal{P} = \bar{W}(U)\bar{\omega}(U)\Delta U / \sum_C W(C) \simeq \Delta U/U_{\text{max}}$. Assuming that the configurations are independent (see below), one has for its variance

$$\mathrm{Var}[\mathcal{N}(U)] = \left(S/\bar{W}(U)\right)^2 N\mathcal{P}(1-\mathcal{P}) \ . \tag{40}$$

Thus, the (relative) statistical error on $\mathcal{N}(U)$ is simply given by

$$\epsilon = \sqrt{\frac{1-\mathcal{P}}{N\mathcal{P}}} \simeq \sqrt{\frac{1}{N\mathcal{P}}} \ . \tag{41}$$

If the sampled state distribution is more or less uniform, $\mathcal{P}$ will be approximately equal to $1/B$, B being the number of bins in the energy interval. Thus, the (relative) statistical error will be on the order of $\sqrt{B/N}$, i.e. the inverse of the square root of the number of states which have been sampled in that bin (whatever the actual number of states in that bin).

Finally, another fact has to be taken into account when estimating the statistical error on various quantities. Indeed, the successive configurations along the random walk are clearly not statistically independent since each one is generated by moving one particle at most from the previous one; that is, C_{i+1} is likely to be in the neighbourhood of C_i even if the configurations are distributed properly as the walk becomes long. As a result, the above expression of the variance is clearly underestimated. This can be quantified by calculating the auto-correlation function of some estimator, e.g. the energy U_C. In practice, the auto-correlation length L_{corr} can be computed as the number of random steps for which this function becomes reasonably small. Then, when estimating the statistical errors on any quantity, the number of sampled states N has to be replaced by N/L_{corr}, measuring the number of independent sampled configurations during the Monte Carlo run.

B   Implementation of the random spin coupling

The calculation of the spin distribution is simplified since we restrict the method to spherical nuclei here. The orbital angular momentum j becomes thus a good quantum number, allowing us to define subshells. The number of levels having a given total angular momentum J for a particular configuration of subshells can be calculated by finding the number of ways the components j's can couple to J according to usual coupling rules. We show in *i)* how we achieve this coupling in a random manner. However, when we treat two (or more) identical nucleons in a same subshell, the restrictions imposed by the Pauli exclusion principle for fermions complicate this coupling, as explained in *ii)*. Note that we do not have to construct explicitly the eigenfunctions of J^2 by use of the Clebsch-Gordan or fractional parentage coefficients, as the method only serves to determine the correct number of states with their good spin. As a matter of fact, we make an arbitrary correspondence between the $|m_1 m_2 \cdots\rangle$ states and the $|JM\rangle$ states. We simply choose at random the $|m_1 m_2 \cdots\rangle$ states so that the corresponding $|JM\rangle$ states are sampled with the correct statistical weights. Thus, we do not calculate an intermediate M-dependent state density $\omega(U, M)$ in order to deduce $\rho(U, J)$ through the usual relation $\rho(U, J) = \omega(U, M = J) - \omega(U, M = J+1)$, as in ref. [23]. Rather, we calculate directly the spin distribution, which allows to properly incorporate pairing effects.

i) Spin coupling for different orbitals:
    Let us show how to couple randomly the spins of the different subshells (for neutrons or protons). As mentioned in Section 2.3, we use the following relation for the coupling of two spins (j_1 and j_2) to a total spin J:

$$J = j_1 + j_2 - \min(d_1, d_2) \; , \tag{42}$$

where d_1 and d_2 are discrete random variables uniformly distributed in $[0, 2j_1]$ and $[0, 2j_2]$, respectively. This relation yields a total spin J obeying the usual coupling rule of angular momentum for independent particles, with adequate weights (i.e., the sampling probability of each spin is proportional to its degeneracy).

In order to prove this, let us calculate the probability distribution of the random variable J defined by equation (42). Since d_1 and d_2 are uniformly distributed, they have the following cumulative distribution functions:

$$F_1(d_1) \;=\; \begin{cases} \dfrac{d_1+1}{2j_1+1} & \text{if } 0 \le d_1 \le 2j_1 \,, \\ 1 & \text{if } d_1 > 2j_1 \,, \end{cases} \tag{43}$$

$$F_2(d_2) \;=\; \begin{cases} \dfrac{d_2+1}{2j_2+1} & \text{if } 0 \le d_2 \le 2j_2 \,, \\ 1 & \text{if } d_2 > 2j_2 \,. \end{cases} \tag{44}$$

Let us define the random variable $d = \min(d_1, d_2)$, and let us determine its cumulative distribution function $F(d)$ using

$$\begin{aligned} F(d) \;&=\; \text{Prob}\left[\min(d_1, d_2) \le d\right] \\ &=\; \text{Prob}\left[(d_1 \le d) \text{ or } (d_2 \le d)\right] \\ &=\; 1 - \text{Prob}[d_1 > d] \,\cdot\, \text{Prob}[d_2 > d] \\ &=\; F_1(d) + F_2(d) - F_1(d) \cdot F_2(d) \,, \end{aligned} \tag{45}$$

where we have used the fact that d_1 and d_2 are independent random variables. Thus, if d reaches the maximum value of either d_1 or d_2 (i.e., $2j_1$ or $2j_2$ respectively), one has $F_1(d) = 1$ or $F_2(d) = 1$, so that

$$F(d) \equiv 1 \qquad \text{if } d \ge \min(2j_1, 2j_2) \,. \tag{46}$$

This implies that the probability of having $d > \min(2j_1, 2j_2)$ is equal to zero, so that J cannot be less than $j_1 + j_2 - \min(2j_1, 2j_2) = |j_1 - j_2|$, as expected. Using equations (43), (44) and (45) we can calculate the probability distribution $f(d)$ of the random variable d as

$$\begin{aligned} f(d) \;&=\; F(d) - F(d-1) \\ &=\; \frac{2(j_1 + j_2 - d) + 1}{(2j_1 + 1)(2j_2 + 1)} \qquad \text{with } 0 \le d \le \min(2j_1, 2j_2) \,. \end{aligned} \tag{47}$$

Thus, the probability distribution of J is simply given by

$$\begin{aligned} \Phi(J) \;&=\; f(j_1 + j_2 - J) \\ &=\; \frac{(2J + 1)}{(2j_1 + 1)(2j_2 + 1)} \qquad \text{with } |j_1 - j_2| \le J \le j_1 + j_2 \,, \end{aligned} \tag{48}$$

which exactly corresponds (within a multiplicative factor) to the statistical weight of the spin J. Note that the denominator comes from the normalization condition

$$\sum_{J=|j_1-j_2|}^{j_1+j_2} \Phi(J) = 1 \tag{49}$$

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of the probability distribution $\Phi(J)$. This procedure can be obviously generalized for the coupling of n independent spins by applying relation (42) recursively.

ii) Identical nucleons in a single orbital:

For identical nucleons in a subshell, only those states are permitted for which the Pauli exclusion principle is obeyed. Thus, the Monte Carlo implementation of the spin coupling is not straightforward, as for different orbitals (case i). A rapid method for handling this problem is to put the required spin distribution in a table. This table, constructed according to the Mayer-Jensen table [22, 45], yields the number of times each spin J occurs for various configurations $(j)^k$, where j is the spin of the subshell and k is the number of identical nucleons occupying the subshell.

As an example, we present in Table 1 a list of the possible angular momenta J for an orbital $j = 9/2$. Note that the multiplicity of the states due to the degeneracy for M is taken into account. The states are labelled by the seniority quantum number s (corresponding to the number of unpaired particles in the orbital), with

$$
\begin{aligned}
s &= 0, 2, 4, \cdots \min(k, 2j + 1 - k) &&\text{for } k \text{ even }, \\
s &= 1, 3, 5, \cdots \min(k, 2j + 1 - k) &&\text{for } k \text{ odd }.
\end{aligned}
\tag{50}
$$

For instance, the various spins of the two-particles states ($k = 2$) are obtained by summing the rows $s = 0$ and $s = 2$ in Table 1. The last column in Table 1 shows the total multiplicity of the states of seniority s. Note that when the subshell is more than half filled (i.e., when $k > j + 1/2$), one applies the same procedure with the number of holes $2j + 1 - k$. Our Monte Carlo procedure to give the spin of a configuration $(j = 9/2)^2$ consists in choosing at random one of the values $J=0, 2, 4, 6, 8$ with the corresponding probabilities 1/45, 5/45, 9/45, 13/45, 17/45. The total weight (needed to normalize the probabilities) is simply $1 + 44 = 45 = \binom{10}{2}$. At the same time, the seniority s is chosen equal 0 or 2 according to the probabilities 1/45, 44/45. The value of the seniority s yields the number of unpaired particles in the considered subshell, needed when treating the pairing interaction (see Section 4). The same table for different values of j has been computed, and an analog procedure is used to yield a (random) spin for all the orbitals.

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Tables

J	0	1	2	3	4	5	6	7	8	9	10	11	12	Total
$s=0$	1													1
$s=2$			5		9		13		17					44
$s=4$	1		5	7	18	11	26	15	17	19	21		25	165
J	1/2	3/2	5/2	7/2	9/2	11/2	13/2	15/2	17/2	19/2	21/2	23/2	25/2	Total
$s=1$					10									10
$s=3$		4	6	8	10	12	14	16	18		22			110
$s=5$	2		6	8	10	12	14	16	18	20			26	132

Table 1: List of the statistical weights of the possible states for different values of spin J and seniority s in a $j = 9/2$ subshell. The upper panel corresponds to states with an even number of particles k ($s = 0, 2, \cdots k$), while the lower panel corresponds to states with odd k ($s = 1, 3, \cdots k$).

Figure captions

Figure 1:   Cumulative state density for ^{56}Fe. The solid line represents the total (with both parities) density, while the positive- and negative-parity densities are represented by dashed and dash-dotted lines, respectively. The dotted line corresponds to the cumulative number of sampled states. The adopted size of the sample is $N = 10^6$.

Figure 2:   Spin distribution (normalized to 1) of the excited levels in the energy interval [20–21 MeV] for ^{56}Fe. The squares represent the results of our Monte Carlo procedure, while the solid line represents those of a direct counting calculation [48]. Both calculations were made using the same single-particle level scheme [46]. The triangles and the crosses correspond, respectively, to the Monte Carlo positive- and negative-parity spin distribution. A sample size $N = 50 \times 10^6$ is adopted.

Figure 3:   Distribution of the excited state angular momentum projection M and of the excited level spin J for ^{56}Fe in the energy interval [8–10 MeV]. The squares correspond to $\omega(U, M)$ resulting from our Monte Carlo calculation, while the solid line represents the gaussian distribution from eq. (20). The triangles stand for the Monte Carlo derived $\rho(U, J)$, while the dashed line represents the asymptotic distribution from the statistical model (eq. 21). The derived value for the effective spin cut-off parameter is $\sigma^2 \simeq 18.8$.

Figure 4: Cumulative parity asymmetry A as a function of excitation energy U for ^{56}Fe. The dotted line represents the result of our Monte Carlo procedure, while the solid line represents those of a direct counting [48]. Note that, for the sake of emphasizing the small discrepancies between both curves, we have slightly shifted the dotted curve to the right. Both calculations were made using the same single-particle level scheme [46].

Figure 5: State density for ^{56}Fe (a) and ^{140}La (b). The solid line represents the combinatorial state density obtained with our Monte Carlo method, plotted in bins of 100 keV, while the dashed line corresponds to the statistical model calculation [49] using the same spectrum of single-particle levels (from [46]). The statistical curve appears as an averaged combinatorial state density.

Figure 6: Comparison of the effective spin cut-off parameter σ^2 as a function of energy U, for ^{120}Sn, ^{162}Dy, and ^{208}Pb. The symbols represent the values derived from our Monte Carlo method (each symbol corresponds to a Monte Carlo simulation), while the solid lines stand for the predictions of the statistical model [49]. Both evaluations have been obtained making use of the same Woods-Saxon single-particle level scheme. This figure is taken from [50].

Figure 7: Cumulative state density including pairing effects derived with our Monte Carlo method for two isobar ($A = 142$) nuclei, as a function of excitation energy U. The solid and the dash-dotted line correspond, respectively, to the case of ^{142}Nd and ^{142}Pr, while the dashed and the dotted lines represent the cumulative state density for both nuclei in the absence of pairing. We took the single-particle level schemes and the pairing strength parameters from ref. [46] (i.e., $G_n \simeq 0.10$ MeV and $G_p \simeq 0.11$ MeV for both nuclei).

a) ^{56}Fe

b) ^{140}La

$\omega(U)$ [MeV^{-1}]

U [MeV]